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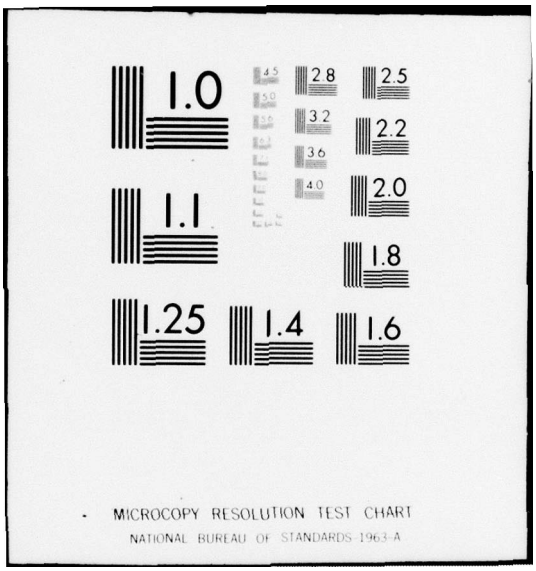
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DISTRIBUTION-FREE PERFORMANCE BOUNDS WITH THE RESUBSTITUTION ERROR ESTIMATE

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Probability inequalities are given for the deviation of the resubstitution error estimate from the unknown conditional probability of error. The inequalities are distribution-free and can be applied to linear discrimination rules, to nearest neighbor rules with a reduced sample size, and to histogram rules.

1. Introduction

The discrimination problem may be formulated as follows. The statistician collects data $(X_1,\theta_1),\ldots,(X_n,\theta_n)$, a sequence of *independent identically distributed* random vectors drawn from the distribution of (X,θ), a random vector independent of the data. For each $1 \le i \le n$, the observation X_i takes values in $\mathbb{R}^m$ and its state θ_i takes values in $\{1,\ldots,M\}$. The discrimination problem is that of estimating the state θ from the data and the observation X using procedures which do not require complete knowledge of the distribution of (X,θ). If $\hat{\theta}$ denotes the estimate, that is, $\hat{\theta} = g(X,V_n)$ where g is a Borel measurable $\{1,\ldots,M\}$-valued function of X and the data $V_n = (X_1,\theta_1,\ldots,X_n,\theta_n)$, then a measure of the performance of the procedure given the data is $L_n = P\{\hat{\theta} \neq \theta | V_n\}$, the conditional probability of error.

Since the distribution of (X,θ) is unknown, there is in general no way of computing L_n from the data. Using the data the statistician may try to estimate L_n by $\hat{L}_n$. A survey of estimation techniques can be found in Toussaint.[1] One of the oldest estimates is the resubstitution estimate

$$\hat{L}_n = n^{-1} \sum_{i=1}^{n} I_{\{\hat{\theta}_i \neq \theta_i\}}$$

where $\hat{\theta}_i = g(X_i,V_n)$, $1 \le i \le n$, are the estimates of the states of $X_1,\ldots,X_n$ with the given discrimination procedure, and where I is the indicator function.

In this paper we obtain upper-bounds for $P\{|L_n-\hat{L}_n| \ge \epsilon\}$ that do not depend upon the distribution of (X,θ), and that are applicable to three large classes of discrimination rules,

(i) the linear discrimination rules,
(ii) the nearest-neighbor rules with reduced sample size, and
(iii) the histogram decision rules.

The existence of distribution-free bounds with the resubstitution estimate for linear discrimination rules was first noticed by Vapnik and Chervonenkis.[10] The bounds for the class (i) improve the bounds given in Devroye and Wagner[2], while the results for the rules (ii) and (iii) are new. The possible existence of distribution-free bounds for (ii) was suggested to the authors by Dr. Penrod[16].

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2. Main Results

Let $\phi_0, \phi_1,\ldots,\phi_{m'}$ be known measurable mappings from $\mathbb{R}^m$ to $\mathbb{R}$ where $m' \ge 1$ and $m \ge 1$, and $\phi_0 \equiv 1$. Let $w_0 = (w_{10},\ldots,w_{1m'}),\ldots, w_M = (w_{M0},\ldots,w_{Mm'})$ be Borel-measurable $\mathbb{R}^{m'+1}$-valued vector functions of the data V_n. Then, the rule which assigns the state $\hat{\theta} = j$ $(1 \le j \le M)$ to X whenever j is the first integer for which

$$\sum_{i=0}^{m'} w_{ji}(V_n)\,\phi_i(X) = \max_{1\le k\le M} \{\sum_{i=0}^{m'} w_{ki}(V_n)\,\phi_i(X)\}$$

is called a linear discrimination rule (see Duda and Hart[3] for a survey of the literature on linear discrimination). We emphasize that the $w_1,\ldots,w_M$ may be picked in an arbitrary fashion, using any method that can or cannot be found in the literature. The functions ϕ_i are picked in advance. The following bound is proved in the Appendix.

Theorem 1. For every $\epsilon > 0$ and for all linear discrimination rules with given $\phi_0,\phi_1,\ldots,\phi_{m'}$, the resubstitution estimate $\hat{L}_n$ satisfies

$$P\{|L_n-\hat{L}_n| \ge \epsilon\} \le 4M(1+(2n)^{m'})^{M-1} e^{-n\epsilon^2/8M^2}.$$

For the interesting case that M=2, we see that

$$P\{|L_n-\hat{L}_n| \ge \epsilon\} \le 8(1+(2n)^{m'})\, e^{-n\epsilon^2/32}.$$

Using the Borel-Cantelli lemma and Theorem 1, we see that for a given m' and M, and uniformly over all linear discrimination rules, $|L_n-\hat{L}_n| \overset{n}{\to} 0$ with probability one, a result due to Glick[11]. Thus, the statistician could pick the $w_1,\ldots,w_M$ that minimize the resubstitution estimate $\hat{L}_n$ because he knows from Theorem 1 that the corresponding probability of error L_n will be very close to $\hat{L}_n$, and that for large n, minimizing $\hat{L}_n$ is nearly equivalent to minimizing L_n (see Wagner[12]).

In the literature special attention has been given to the nearest-neighbor rule with a reduced number of observations where the reduction is a result of editing (see for instance Wilson[4]), condensing (Hart[5]) or any other operation (Tomek[6]). In general, we end up with $\mathbb{R}^m \times \{1,\ldots,M\}$-valued random vectors $(Y_1,\xi_1),\ldots,(Y_K,\xi_K)$ where K is an integer-valued random variable with $1 \le K \le k_n$. The (Y_i,ξ_i) and K may depend upon the data in an arbitrary fashion. A new observation X is assigned the state $\hat{\theta} = \xi_j$ whenever j is the smallest index for which

$$\|X-Y_j\| = \min_{1\le i\le K} \|X-Y_i\| .$$

Thus, $\hat{\theta}$ is the state of the nearest neighbor to X among $Y_1,\ldots,Y_K$. In the Appendix the following Theorem is proved.

Theorem 2. For every $\epsilon > 0$, and for all the nearest-neighbor rules with reduced sample size, the resubstitution estimate $\hat{L}_n$ satisfies

$$P\{|L_n-\hat{L}_n| \ge \epsilon\} \le 4M(1+(2n)^m)^{k_n-1} e^{-n\epsilon^2/8k_n^2}$$

where k_n is an upper-bound on the reduced sample size.

We remark that this bound is independent of the distribution of (X,θ). The bound converges to 0 as n grows large provided that the sequence $k_1,k_2,\ldots$ is picked in such a way that $k_n^3 \log n/n \overset{n}{\to} 0$. It is clear that this bound is useless for the well-known nearest neighbor rule[7], that is, the rule with $K=k_n=n$ and $(Y_i,\xi_i) = (X_i,\theta_i)$, $1\le i\le n$. This was to be expected because the resubstitution estimate with the nearest-neighbor rule is overly optimistic. In fact, if the probability measure μ of X is absolutely continuous with respect to Lebesgue measure, then $\hat{L}_n = 0$ with probability one, no matter what value L_n takes.

Theorem 2 can be useful for reduced, selective, condensed or edited nearest-neighbor rules[4-6,13-14]. If k_n is a prespecified number of (Y_i,ξ_i)'s that are to be used in the new nearest-neighbor rule, then the statistician could compute $\hat{L}_n$ with some selected data $(X_{i_1},\theta_{i_1}),\ldots,(X_{i_{k_n}},\theta_{i_{k_n}})$ where $\{i_1,\ldots,i_{k_n}\}$ is a subset of $\{1,\ldots,n\}$, and decide to use that set of indices for which the resubstitution estimate is minimal. Using Theorem 2, we also know how much confidence we can put in our estimate $\hat{L}_n$ regardless of the selection procedure of the (Y_i,ξ_i) and without any knowledge of the distribution of (X,θ).

The (Y_i,ξ_i), $1\le i\le k_n$, partition $\mathbb{R}^m$ into k_n disjoint sets $A_1,\ldots,A_{k_n}$ where the state of X is estimated by $\hat{\theta} = \xi_j$ whenever X takes values in A_j (that is, X is closest to Y_j). The partition in this case depends on the data because the Y_i depend upon the data. For a given fixed partition of $\mathbb{R}^m$, we can expect to obtain tighter upper-bounds for $P\{|L_n-\hat{L}_n| \ge \epsilon\}$ even if the partition is not generated by a reduced nearest-neighbor rule.

Let $A_1,\ldots,A_{k_n}$ be <u>any</u> fixed partition of $\mathbb{R}^m$ and let $\xi_1,\ldots,\xi_{k_n}$ be $\{1,\ldots,M\}$-valued random variables where, as before, ξ_j is the state assigned to X whenwhenever X takes values in A_j. Such rules will be called histogram decision rules. We prove the following four distribution-free inequalities that are valid <u>no matter</u> how the ξ_i depend upon the data. The inequalities do not imply one another.

Theorem 3. For a given k_n-member partition of $\mathbb{R}^m$, for any way of specifying $\xi_1,\ldots,\xi_{k_n}$ from the data in a histogram decision rule, and for every $\epsilon > 0$, the resubstitution estimate $\hat{L}_n$ satisfies

$$P\{|L_n-\hat{L}_n| \ge \epsilon\} \le g_{ni} \quad , \quad 1 \le i \le 4,$$

where

$$g_{n1} = 4\, k_n \min(1+2n,M)\, e^{-n\epsilon^2/8k_n^2}$$

$$g_{n2} = 2\, k_n\, M\, e^{-2n\epsilon^2/M^2k_n^2}$$

$$g_{n3} = 4 \min\left(M^{k_n}, 2^{2n}, (4n/k_n)^{k_n}\right) e^{-n\epsilon^2/8}$$

$$g_{n4} = 2\, M^{k_n}\, e^{-2n\epsilon^2/M^{2k_n}} .$$

We note here that g_{n1} and g_{n3} are useful even if $M = \infty$ (i.e., the ξ_i and θ_i can take a countably infinite number of values). Clearly, all the g_{ni} are independent of the dimension m and the distribution of (X,θ), and $g_{n3} \overset{n}{\to} 0$ provided that $k_n/n \overset{n}{\to} 0$. If $k_n = \infty$, the bounds are not applicable, and, as we will see, the resubstitution estimate does not possess the distribution-free properties that it has with finite partitions of $\mathbb{R}^m$. Assume that $A_1,A_2,\ldots$ is a fixed countably infinite partition of $\mathbb{R}^m$. If the ξ_i are random variables that are independent of the data, then

$$P\{|L_n-\hat{L}_n| \ge \epsilon\} \le 2e^{-2n\epsilon^2} \qquad (1)$$

for any $\epsilon > 0$. However, such rules are impractical. The closest one can come to the Bayes rule with a fixed partition is to let $\xi_i = j$ if j is the smallest integer such that $N_{ij} = \max_{1\le \ell\le M} N_{i\ell}$ where N_{ij} is the number of (X_k,θ_k)'s with $X_k \in A_i$ and $\theta_k = j$. But even with this obvious choice of $\xi_1,\xi_2,\ldots$ we see that for any m and $M \ge 2$, there always exists a distribution of (X,θ) such that $|L_n-\hat{L}_n| \ge \frac{1}{2}$ with probability one. Indeed, assume that M=2, that $\theta=2$ with probability one, and that X takes values in each $A_1,\ldots,A_{2n}$ with equal probability $1/2n$. If the ξ_i are picked as described, then the resubstitution estimate $\hat{L}_n$ equals 0. Furthermore,

$$L_n = \sum_{i=1}^{2n} P\{X\in A_i\}\, I_{\{N_{i2}=0\}} \ge n/2n = 1/2.$$

This shows that even with the most obvious dependency of the ξ_i on the data, we will never be able to upper-bound $P\{|L_n-\hat{L}_n| \ge \epsilon\}$ by an expression that decreases to 0 as n grows large, uniformly over all distributions of (X,θ).

3. Appendix

Proof of Theorem 1.

Let ν be the probability measure of (X,θ) where X takes values in $\mathbb{R}^{m'}$ and θ takes values in $\{1,\ldots,M\}$. It is clear that if ν_n is the empirical measure for $(X_1,\theta_1),\ldots,(X_n,\theta_n)$, and if $A_1,\ldots,A_M$ is the partition of $\mathbb{R}^{m'}$ that is generated by the linear discrimination rule (that is, A_i is the set on which we estimate the state of X by i), then

$$L_n = \sum_{i=1}^{M} \nu(A_i \times \{i\}^c)$$

and

$$\hat{L}_n = \sum_{i=1}^{M} \nu_n(A_i \times \{i\}^c) .$$

Thus,

$$|L_n - \hat{L}_n| = \left|\sum_{i=1}^{M} (\nu(A_i\times\{i\}^c) - \nu_n(A_i\times\{i\}^c))\right|$$

$$= \left|\sum_{i=1}^{M} (\nu_n(A_i\times\{i\}) - \nu_n(A_i\times\{i\}))\right|$$

$$\le M \sup_{\substack{A\in\mathcal{A} \\ i\in\{1,\ldots,M\}}} |\nu_n(A\times\{i\}) - \nu(A\times\{i\})|$$

where $\mathcal{A}$ is the class of all sets that are intersections of $(M-1)$ linear halfspaces of $\mathbb{R}^{m'}$. We recall that a linear halfspace of $\mathbb{R}^{m'}$ is a set of $x = (x^1,\ldots,x^{m'})$ for which $x^1a_1 + \ldots + x^{m'}a_{m'} \ge a_0$ or $x^1a_1 + \ldots + x^{m'}a_{m'} < a_0$ for some $(a_0,a_1,\ldots,a_{m'}) \in \mathbb{R}^{m'+1}$. Thus, every $(a_0,a_1,\ldots,a_{m'})$ defines two linear halfspaces.

By an inequality of Vapnik and Chervonenkis[9],

$$P\{|L_n-\hat{L}_n| \ge \epsilon\}$$

$$\le P\{\sup_{\substack{A\in\mathcal{A} \\ 1\le i\le M}} |\nu_n(A\times\{i\}) - \nu(A\times\{i\})| \ge \epsilon/M\}$$

$$\le 4s(\mathcal{B},2n)e^{-n(\epsilon/M)^2/8}$$

where $\mathcal{B} = \mathcal{A}\times\{\{1\},\ldots,\{M\}\}$ and $s(\mathcal{B},n)$ is the maximum over all $(x_1,y_1),\ldots,(x_n,y_n)$ in $\mathbb{R}^{m'}\times\{1,\ldots,M\}$ of the number of different sets in $\{\{(x_1,y_1)\}\cup\ldots\cup\{(x_n,y_n)\} \cap B \mid B\in\mathcal{B}\}$. If $\mathcal{A}$ is the class of all linear halfspaces of $\mathbb{R}^{m'}$ and $M=1$, then $s(\mathcal{B},n) \le 1+n^{m'}$ by a theorem of Cover[8] (see also Vapnik and Chervonenkis[9]). It is clear that if $\mathcal{A}$ is the class of all intersections of M^*-1 or less linear halfspaces and $M=1$, then $s(\mathcal{B},n) \le (1+n^{m'})^{M^*-1}$. If $M>1$, then $s(\mathcal{B},n) \le M(1+n^{m'})^{M^*-1}$. Indeed, if s_1 is the number of different sets in $\{\{x_1\}\cup\ldots\cup\{x_n\}\cap A \mid A\in\mathcal{A}\}$, then the number of different sets in $\{\{(x_1,y_1)\}\cup\ldots\cup\{(x_n,y_n)\}\cap B \mid B\in\mathcal{A}\times\{\{1\},\ldots,\{M\}\}\}$ is at most Ms_1. Thus we have shown that

$$P\{|L_n - \hat{L}_n| \ge \epsilon\} \le 4M(1+(2n)^{m'})^{M-1} e^{-n\epsilon^2/8M^2} .$$

Q.E.D.

Proof of Theorem 2.

Let us use the notation of Theorem 1 where we let $A_1,\ldots,A_K$ be the partition of $\mathbb{R}^m$ that is generated by the nearest-neighbor rule with $(Y_1,\xi_1),\ldots,(Y_K,\xi_K)$ (i.e., A_i is the set on which we estimate the state of X by ξ_i and for which Y_i is the nearest neighbor to X among $Y_1,\ldots,Y_K$), then

$$L_n = \sum_{i=1}^{K} \nu(A_i\times\{\xi_i\}^c)$$

and

$$\hat{L}_n = \sum_{i=1}^{K} \nu_n(A_i\times\{\xi_i\}^c) .$$

Thus, arguing as in Theorem 1, we have

$$|L_n-\hat{L}_n| \le K \sup_{\substack{A\in\mathcal{A} \\ 1\le i\le M}} |\nu_n(A\times\{i\}) - \nu(A\times\{i\})|$$

where $\mathcal{A}$ is the class of all sets that are intersections of (k_n-1) or less linear halfspaces of $\mathbb{R}^m$. Since $K \le k_n$, we have by the argument of Theorem 1 that

$$P\{|L_n-\hat{L}_n|\ge\epsilon\} \le 4M(1+(2n)^m)^{k_n-1} e^{-n\epsilon^2/8k_n^2} .$$

Q.E.D.

Proof of Theorem 3.

It is clear that

$$|L_n-\hat{L}_n| = |\nu(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\xi_\ell\}^c)) - \nu_n(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\xi_\ell\}^c))|$$

$$= |\nu(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\xi_\ell\})) - |\nu_n(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\xi_\ell\}))|$$

$$\le \sum_{\ell=1}^{k_n} \sup_{1\le i\le M} |\nu(A_\ell\times\{i\}) - \nu_n(A_\ell\times\{i\})| .$$

Thus, if $\mathcal{C}_\ell$ is the class of sets of the form $A_\ell\times\{i\}$, $1\le i\le M$, then we know by an inequality of Vapnik and Chervonenkis[9] that

$$P\{|L_n-\hat{L}_n| \ge \epsilon\}$$

$$\le k_n \sup_{1\le\ell\le k} P\{\sup_{C\in\mathcal{C}_\ell} |\nu(C)-\nu_n(C)| \ge \epsilon/k_n\}$$

$$\le 4k_n\left(\sup_{1\le\ell\le k_n} s(\mathcal{C}_\ell,2n)\right)e^{-n(\epsilon/k_n)^2/8}$$

$$\le 4k_n \operatorname{Min}(1+2n,M)\, e^{-n\epsilon^2/8k_n^2} .$$

Also,

$$P\{|L_n-\hat{L}_n| \geq \epsilon\}$$

$$\leq P\left\{\sum_{\ell=1}^{k_n}\sum_{i=1}^{M} |\nu(A_\ell\times\{i\}) - \nu_n(A_\ell\times\{i\})| \geq \epsilon\right\}$$

$$\leq k_n M \sup_{\substack{1\leq i\leq M \\ 1\leq \ell\leq k}} P\{|\nu(A_\ell\times\{i\}) - \nu_n(A_\ell\times\{i\})| \geq \epsilon/k_nM\}$$

$$\leq 2k_nMe^{-2n\epsilon^2/M^2k_n^2}$$

by an inequality of Hoeffding[15]. Furthermore,

$$|L_n-\hat{L}_n|$$

$$\leq \sup_{\text{all } (\lambda_1,\ldots,\lambda_{k_n}) \text{ from } \{1,\ldots,M\}^{k_n}} |\nu(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\lambda_\ell\})) - \nu_n(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\lambda_\ell\}))|$$

so that

$$P\{|L_n-\hat{L}_n|\geq\epsilon\} \leq 4s(\mathcal{D}^*,2n)\, e^{-n\epsilon^2/8}$$

where $\mathcal{D}^*$ is the class of all sets of the form $\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\lambda_\ell\})$ where $(\lambda_1,\ldots,\lambda_{k_n})\in\{1,\ldots,M\}^{k_n}$. Clearly, $s(\mathcal{D}^*,2n) \leq 2^{2n}$ for all k_n. However, if $k_n < 2n$, then $s(\mathcal{D}^*,2n) \leq M^{k_n}$ and, in general, we must have that $s(\mathcal{D}^*,2n) \leq 2^{k_n}(2n/k_n)^{k_n}$. This proves the inequality with g_{n3}.

Finally, notice that

$$P\{|L_n-\hat{L}_n| \geq \epsilon\}$$

$$\leq \sum_{d\in\mathcal{D}} P\{|\nu(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\lambda_\ell\})) - \nu_n(\bigcup_{\ell=1}^{k_n}(A_\ell\times\{\lambda_\ell\}))| \geq \epsilon/Mk_n\}$$

$$\leq 2M^{k_n} e^{-2n\epsilon^2/M^{2k_n}}.$$

Q.E.D.

Proof of (1).

Inequality (1) is a corollary of Hoeffding's inequality[15] if we note that $|L_n-\hat{L}_n| = |\nu(C)-\nu_n(C)|$ where

$$C = \bigcup_{\ell=1}^{\infty}(A_\ell\times\{\xi_\ell\}^c).$$

Q.E.D.

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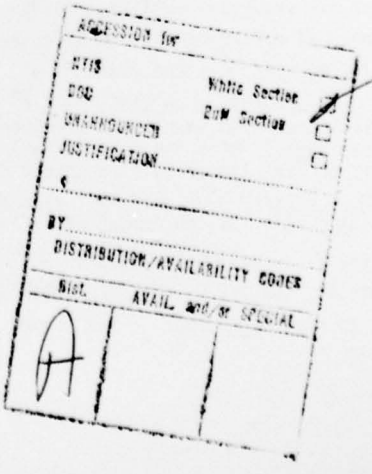

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